Application Serial No. 09/506,717
Amendment dated April 23, 2004
Reply to Office Action dated October 23, 2003

Claims

Claims 1-4 (canceled).

Claim 5 (currently amended). A method for use in deriving fixed bond information, comprising:

analyzing a ~~Kekulé structure~~ delocalized representation of a chemical structure, wherein at least a portion of the delocalized structure representation describes a polycyclic ring system;

identifying, based on valence information, a plurality of fixed bond representation candidates for at least a portion of the chemical structure;

evaluating at least a subset of the fixed bond representation candidates;

selecting from among the plurality of fixed bond representation candidates based on the evaluation; and

producing fixed bond information based on the selection;

~~wherein at least a portion of the Kekulé structure representation describes a polycyclic ring system.~~

Claim 6 (currently amended). The method of claim 5, wherein at least a portion of the ~~Kekulé structure~~ delocalized representation describes a ring system with a hetero substitution pattern.

Claim 7 (currently amended). The method of claim 5, wherein at least a portion of the ~~Kekulé structure~~ delocalized representation describes a non-cyclic system.

Claim 8 (currently amended). The method of claim 5, wherein at least a portion of the ~~Kekulé structure~~ delocalized representation describes an acyclic system.

Claim 9. (currently amended). A method for use in deriving fixed bond information, comprising:

analyzing a ~~Kekulé structure~~ delocalized representation of a chemical structure;

identifying, based on valence information, a plurality of fixed bond representation candidates for at least a portion of the chemical structure;

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evaluating at least a subset of the fixed bond representation candidates;

selecting from among the plurality of fixed bond representation candidates based on the

evaluation;

producing fixed bond information based on the selection; and

based on the fixed bond information, producing a fixed bond representation that includes

a pair of opposite charges lacked by the ~~Kekulé structure~~ delocalized representation.

Claim 10 (currently amended). A method for use in deriving fixed bond information,

comprising:

analyzing a ~~Kekulé structure~~ delocalized representation of a chemical structure;

identifying, based on valence information, a plurality of fixed bond representation

candidates for at least a portion of the chemical structure;

evaluating at least a subset of the fixed bond representation candidates;

selecting from among the plurality of fixed bond representation candidates based on the

evaluation;

producing fixed bond information based on the selection; and

based on the fixed bond information, producing a fixed bond representation that includes

a pair of radicals lacked by the Kekulé structure representation.

Claim 11 (currently amended). The method of claim 5, <u>wherein the step of identifying is</u>

<u>performed based on electronic State and valence distribution (ESVD), and</u> further comprising:

queuing at least a subset of the ~~candidates~~ ESVDs by priority.

Claim 12 (currently amended). A method for use in deriving fixed bond information,

comprising:

analyzing a ~~Kekulé structure~~ delocalized representation of a chemical structure;

identifying, based on valence information, a plurality of fixed bond representation

candidates for at least a portion of the chemical structure;

evaluating at least a subset of the fixed bond representation candidates;

selecting from among the plurality of fixed bond representation candidates based on the

evaluation;

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producing fixed bond information based on the selection; and

using a precomputed table of atom valences as a function of element, charge, radical

state, and number and distribution of bonds inside and outside of a delocalized region in the

~~Kekulé structure~~ delocalized representation.

Claim 13 (original). The method of claim 12, wherein the table is configured to allow

additional elements and values to be added.

Claim 14 (original). The method of claim 12, wherein the table is configured to allow

additional elements and values to be added to apply to any chemical element.

Claim 15 (currently amended). The method of claim 5, further comprising:

deriving electronic state and valence distributions information together with analyzing the

~~Kekulé structure~~ delocalized representation.

Claim16 (currently amended). The method of claim 5, further comprising:

determining whether it is ~~practical~~ possible to produce a neutral, non-radical fixed bond

representation of the most chemical ~~structure~~ structures.

Claims 17 and 18 (Canceled).

Claim 19 (currently amended). The method of claim 5, wherein at least a portion of the

~~Kekulé structure~~ delocalized representation describes a monocyclic ring system.

Claim 20 (currently amended). A system for use in deriving fixed bond information,

comprising:

an analyzer analyzing a ~~Kekulé structure~~ delocalized representation of a chemical

structure, wherein at least a portion of the delocalized representation describes a polycyclic ring

system;

an identifier identifying, based on valence information, a plurality of fixed bond

representation candidates for at least a portion of the chemical structure;

an evaluator evaluating at least a subset of the fixed bond representation candidates;

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a selector electing from among the plurality of fixed bond representation candidates based on the evaluation; and

a producer producing fixed bond information based on the selection;̲.

~~wherein at least a portion of the Kekulé structure representation describes a polycyclic ring system.~~

Claim 21 (currently amended). Computer software, residing on a computer-readable storage medium, comprising a set of instructions for use in a computer system to help cause the computer system to derive fixed bond information, the instructions causing the system to:

analyze a ~~Kekulé structure~~ d̲e̲l̲o̲c̲a̲l̲i̲z̲e̲d̲ representation of a chemical structure, ̲w̲h̲e̲r̲e̲i̲n̲ ̲a̲t̲ l̲e̲a̲s̲t̲ ̲a̲ ̲p̲o̲r̲t̲i̲o̲n̲ ̲o̲f̲ ̲t̲h̲e̲ ̲d̲e̲l̲o̲c̲a̲l̲i̲z̲e̲d̲ ̲r̲e̲p̲r̲e̲s̲e̲n̲t̲a̲t̲i̲o̲n̲ ̲d̲e̲s̲c̲r̲i̲b̲e̲s̲ ̲a̲ ̲p̲o̲l̲y̲c̲y̲c̲l̲i̲c̲ ̲r̲i̲n̲g̲ ̲s̲y̲s̲t̲e̲m̲;

identify, based on valence information, a plurality of fixed bond representation candidates for at least a portion of the chemical structure;

evaluate at least a subset of the fixed bond representation candidates; ~~and~~

select from among the plurality of fixed bond representation candidates based on the evaluation; and

produce fixed bond information based on the selection;̲.

~~wherein at least a portion of the Kekulé structure representation describes a polycyclic ring system.~~

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